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March 27, 2002

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This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

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The Multi-scale Model Approach to Thermohydrology at Yucca Mountain

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Abstract

The Multi-Scale Thermo-Hydrologic (MSTH) process model is a modeling abstraction of thermal hydrology (TH) of the potential Yucca Mountain repository at multiple spatial scales. The MSTH model as described herein was used for the Supplemental Science and Performance Analyses (BSC, 2001) and is documented in detail in CRWMS M&O (2000) and Glascoe et al. (2002). The model has been validated to a nested grid model in Buscheck et al. (In Review). The MSTH approach is necessary for modeling thermal hydrology at Yucca Mountain for two reasons: (1) varying levels of detail are necessary at different spatial scales to capture important TH processes and (2) a fully-coupled TH model of the repository which includes the necessary spatial detail is computationally prohibitive. The MSTH model consists of six 'submodels' which are combined in a manner to reduce the complexity of modeling where appropriate. The coupling of these models allows for appropriate consideration of mountain-scale thermal hydrology along with the thermal hydrology of drift-scale discrete waste packages of varying heat load. Two stages are involved in the MSTH approach, first, the execution of submodels, and second, the assembly of submodels using the Multi-scale Thermohydrology Abstraction Code (MSTHAC). MSTHAC assembles the submodels in a five-step process culminating in the TH model output of discrete waste packages including a mountain-scale influence.

Introduction

There are many challenges facing the modeling of thermal hydrology (TH) at the potential Yucca Mountain repository. Repository performance measures depend on TH behavior within a few meters of the emplacement drifts as well as on thermal and TH behavior on a repository (or mountain) scale. In order to capture these processes an appropriate TH model needs to consider a 'mountain scale' as well as a 'drift scale'. The two are needed as a mountain scale model alone will smear important TH processes occurring at the drift while a drift scale model will not be able to appropriately capture the three dimensionality of heat flow and repository edge effects.

Three approaches to modeling TH at both a mountain-scale and a drift-scale are possible. The first approach is a 'brute force approach' where the whole mountain is modeled by a single TH model with detail at the drift. This method is simply too computationally demanding. A second approach is the use of an embedded model often referred to as a 'telescoped model' where a detailed drift-scale model is embedded within a coarser and less detailed mountain-scale model. This approach is also too computationally demanding when considering the number of realizations necessary to consider parameter sensitivity and variation in waste package placement within the drift. A third approach to modeling TH at both the mountain-scale and at the drift-scale is through the use of a multiple scale analysis where a rapid analysis of TH at different spatial scales can be achieved under appropriate simplifying assumptions. This third approach is the approach of the MSTH model.

The MSTH model was developed to rapidly analyze TH at Yucca Mountain thus allowing for variability in waste package placement and heat loading as well as allowing for a comprehensive parameter sensitivity analysis. The MSTH model assumes the following:

- Hydrologic processes are only important at the drift scale.
- Conduction is the only heat process important at the mountain scale.
- Due to the linear nature of conduction, temperature can be mapped between drift and mountain scales.

The MSTH approach includes the use of NUFT 3.0s (LLNL, 1999) and the use of the Multi-Scale Thermal-Hydrology Abstraction Code referred to as MSTHAC (LLNL, 2001). To test the appropriateness of these assumptions when modeling TH, the MSTH model of a single drift was validated against a fully-coupled embedded model (Busheck et al., 2002).

MSTH Model Concept

The MSTH approach breaks the solution of Yucca Mountain TH into smaller pieces by varying dimensionality requirements (one-, two-, or three-dimensional) as needed for detail. The MSTH approach subdivides the problem into thermal and thermohydrologic submodels. By subdividing the problem, more efficient thermal conduction and radiation submodels are used to address the three-dimensional nature of repository dimensions and waste-package variability. Similarly, a two-dimensional thermohydrologic model is used to model all TH variables in detail within the drift.

MSTH Spatial Scales

Two spatial scales are considered for the MSTH model: (1) a mountain scale (on the order of 100's to 1000's of meters) and (2) a drift-scale (on the order of fraction of meters). Drift-scale modeling includes the coupling of drift-scale processes both within the Engineered Barrier System (EBS) and with the Near Field Environment (NFE). Mountain-scale processes are needed to account for the influence of the ground surface, the water table, and most importantly the influence of repository edge cooling effects. In addition to coupling the drift scale and mountain scale, the MSTH model also allows for consideration of the effect of different waste packages types, e.g., different Commercial Spent Nuclear Fuel (CSNF) waste packages, co-disposal of Defense High Level Waste (DHLW) on the various performance measures.

MSTH Submodels

The MSTH model simulates processes under a range of heat loading conditions to capture the edge effects within the repository and the discrete nature of waste packages.

MSTH simulates at various locations within the domain to account for variations in stratigraphy and infiltration. This is accomplished by simultaneously solving six ‘submodels’ at different spatial scales. These six submodels comprising the MSTH model are categorized into four NUFT submodels (SMT, SDT, DDT, LDTH) and into two MSTHAC submodels (LMDTH, DMTH). A consistent naming convention is used for these submodels. The first letter applies to the *thermal loading* where S is the ‘smeared’ area averaged heat loading, L is the ‘line’ heat loading, and D is the ‘discrete’ point heat loading. The second letter applies to the *spatial scaling* where M is the ‘mountain’ scale and D is the ‘drift’ scale. The last letters refer to the *variables considered* where T indicates that only ‘thermal conduction’ variables are considered and where TH indicates that all ‘thermohydrologic’ variables are considered.

The four different NUFT submodels are solved simultaneously at different spatial scales. These four submodels are the following:

- SMT (Smeared-heat-source, Mountain-scale, Thermal-conduction) Submodel: the 3D smeared-source mountain-scale thermal-only model.
- LDTH (Line-averaged-heat-source, Drift-scale, Thermohydrologic) Submodel: the line-source drift-scale thermal-hydrology model.
- SDT (Smeared-heat-source, Drift-scale Thermal-conduction) Submodel: the 1D smeared-source drift-scale thermal-only model.
- DDT (Discrete-heat-source, Drift-scale Thermal-conduction) Submodel: the 3D discrete-source drift-scale thermal-only model.

The MSTH model processes the four NUFT submodels using MSTHAC to produce the two following submodels:

- LMTH (Smeared-heat-source, Mountain-scale, Thermal-conduction) Submodel: the intermediary 3D line-source mountain-scale thermo-hydrologic model.
- DMTH (Line-averaged-heat-source, Drift-scale, Thermohydrologic) Submodel: the final 3D discrete-source mountain-scale thermo-hydrology model.

Figure 1 illustrates the general conceptual relation between the four NUFT submodels (identified by red text) and the two MSTHAC submodels (identified by blue text). The successive nature of the NUFT submodel execution followed by the MSTHAC calculation for final output is illustrated in the flowchart of Figure 2.

MSTH Model Process

The MSTH model can be subdivided into the two specific ‘stages’ illustrated in Figure 2. Stage 1 is the simultaneous execution of the four NUFT submodels. Stage 2 is the assembly of the NUFT submodel results into final MSTH results through the use of MSTHAC. These processes are discussed in detail below.

MSTH MODEL STAGE 1: NUFT Submodel Execution

At each of 33 locations spaced evenly throughout the repository area, a two-dimensional LDTH submodel solves for thermohydrologic processes (e.g., surface infiltration rates, hydrologic properties). At each location an Areal Mass Loading (AML) curve is generated which describes the temperature history due to a specified heat input to the LDTH model.

The three-dimensional SMT and the one-dimensional SDT submodels solve for thermal conduction only and both share the same smeared-heat-source approximation and thermal-conduction representation of heat flow. The one-dimensional SDT submodel is executed at the same 33 locations and for the same AML’s as the LDTH submodels providing a linkage between the SMT and the LDTH submodels. The common repository location of the SDT submodel temperature and the LDTH submodel drift-wall temperature allows for the SMT submodel temperature to be corrected for both the influence of TH processes on temperature and for the influence of 2-D drift-scale dimensionality (orthogonal to the axis of the drift). This is accomplished by interpolating between AML histories. The SMT, SDT, and LDTH submodels all share a blended heat-generation history of the entire WP repository; hence, the heat-generation history is effectively that of an average WP.

The three-dimensional DDT submodel is a drift-scale submodel which includes individual WP's of distinct heat-generation history. The DDT submodel solves for thermal conduction and accounts for thermal radiation in addition to thermal conduction between the WP's and drift surfaces. The drift-wall temperatures for an average WP, calculated with the combined use of the LDTH, SMT and SDT submodels, are then further modified to account for waste-package-specific deviations using the DDT submodel.

One complete MSTH model simulation requires multiple NUFT submodel executions to simulate the entire repository. Each MSTH simulation includes the following NUFT submodel executions:

- 1 SMT execution
- 2 DDT executions
- 33 SDT locations/AML x 4 AML's = 132 SDT executions
- 33 LDTH locations/AML x 4 AML's = 132 LDTH executions

Specific details of the execution of the NUFT submodels is discussed in detail in the Calculation Report (BSC, 2001b).

MSTH MODEL STAGE 2: MSTHAC assembly process

The use of MSTHAC to assemble the execution results of the NUFT submodels into final output is the second part of the MSTH model (see Figure 2). MSTHAC assembles the execution results from the submodels at the 33 locations within the repository creating time-varying areal mass loading (AML) curves. These results are then interpolated to 671 'locations' for the Higher Temperature Operating Mode (HTOM) repository footprint and to 762 'locations' for the larger Lower Temperature Operating Mode (LTOM) repository footprint for assembly of the LMTH and DMTH submodels (see Figure 3 for the HTOM and LTOM footprints and Figure 4 for the 33 submodel locations).

The MSTHAC approach can be broken into five steps which center on the construction of two time-varying 'areal mass loadings' (AML's): an effective AML (AML_{effective}) and a specific AML (AML_{specific}). The AML_{effective} varies spatially and temporally and is the interpolated AML that would be prescribed for an insulated heat model (SDT) to predict the temperature produced by a mountain-scale model (SMT). The AML_{specific} incorporates the discrete nature of the waste packages using the DDT model. Both AML's are used to interpret LDTH model results to the LMTH and DMTH models. The five step process of MSTHAC is illustrated as an overview in Figure 5. Each step is explained in detail below in conjunction with Figures 6 through 10.

MSTHAC Step 1: Assemble AML_{effective} (Figure 6)

The temperature history from the SDT model is plotted for each of the 33 spatial locations for a 'family' of four AML's (66, 55, 27 and 14 MTU/acre for HTOM; 55, 46, 23 and 11 MTU/acre for LTOM). The temperature results are then spatially interpolated to the 671 locations for HTOM (762 locations for LTOM). Atop the plotted family of SDT temperature histories at each spatial location is plotted the time history of the temperature from the SMT model. The AML_{effective} is interpolated by determining the AML needed for the SDT model to generate the SMT temperature at any given time.

MSTHAC Step 2: Interpolate LMTH (Figure 7)

The LMTH results are determined by taking the TH output from the LDTH models and plotting the time-history of the variables for each of the family of AML's. First for each of the locations (671 for HTOM, 762 for LTOM) the TH output history from the LDTH model is plotted for each of the four AML's. Second, the TH history for the LMTH at any given time t^* is determined by interpolating the TH value at AML_{effective}(t^*) from the LDTH histories.

MSTHAC Step 3: Calculate DMTH (Figure 8)

The discrete TH values are calculated from the LMTH model by incorporating the DDT submodel temperature results. Here the temperature variation along the average temperature of the LMTH model accounts for differences in waste package loading. The temperature difference is calculated using the AML_{effective} and the temperature from the

DDT model. This difference is then superimposed on the LMTH model to yield DMTH model results.

MSTHAC Step 4: Assembling AML_{specific} (Figure 9)

The procedure for assembling AML_{specific} is very similar to that of assembling $AML_{\text{effective}}$. The temperature history from the LDTH model is plotted for each of the 33 spatial locations for a 'family' of four AML's (66, 55, 27 and 14 MTU/acre for HTOM; 55, 46, 23 and 11 MTU/acre for LTOM). The temperature results are then spatially interpolated to the 671 locations for HTOM (762 locations for LTOM). Atop the plotted family of LDTH temperature histories at each spatial location is plotted the time history of the temperature from the DMTH model. The $AML_{\text{effective}}$ is interpolated by determining the AML needed for the LDTH model to generate the DMTH temperature at any given time.

MSTHAC Step 5: Interpolate TH variables for DMTH (Figure 10)

The DMTH results are determined by taking the TH output from the LDTH models and plotting the time-history of the variables for each of the family of AML's. First for each of the locations (671 for HTOM, 762 for LTOM) the TH output history from the LDTH model is plotted for each of the four AML's. The TH history for the DMTH at any given time t^* is determined by interpolating the TH value at $AML_{\text{specific}}(t^*)$ from the LDTH histories.

Multi-scale Model Approach Summary

The MSTH modeling approach can be summarized by the following four points:

1. The multi-scale model is an effective and efficient method for modeling thermal hydrology of the potential Yucca Mountain waste repository.
2. The multi-scale model is currently the only computationally effective way to investigate the large number of realizations required for complete repository analysis.

3. The multi-scale model consists of NUFT submodel execution followed by MSTHAC calculation of T-H variables.
4. MSTHAC involves five simple interpolation and calculation steps to convert NUFT submodel output to thermal-hydrological output for any location in the repository domain.

Acknowledgements

This work was sponsored by the Yucca Mountain Project and performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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Version 6.4.2. 10419-6.4.2-00.

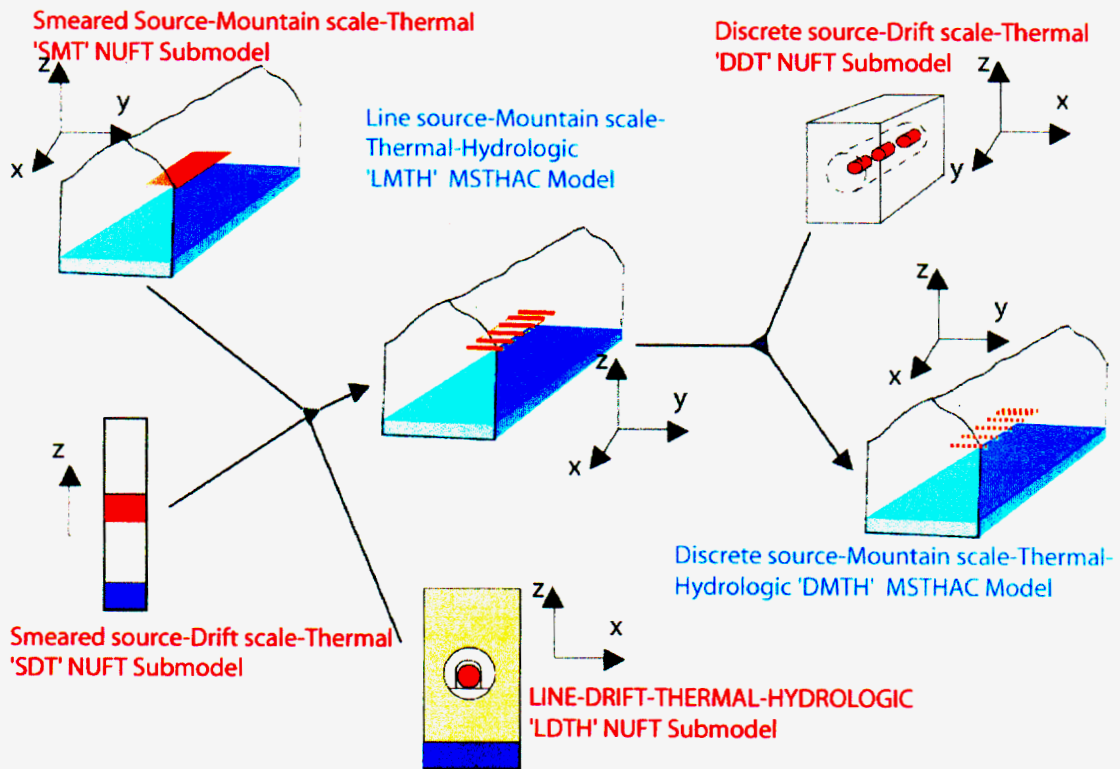


Figure 1. Multi-scale modeling approach.

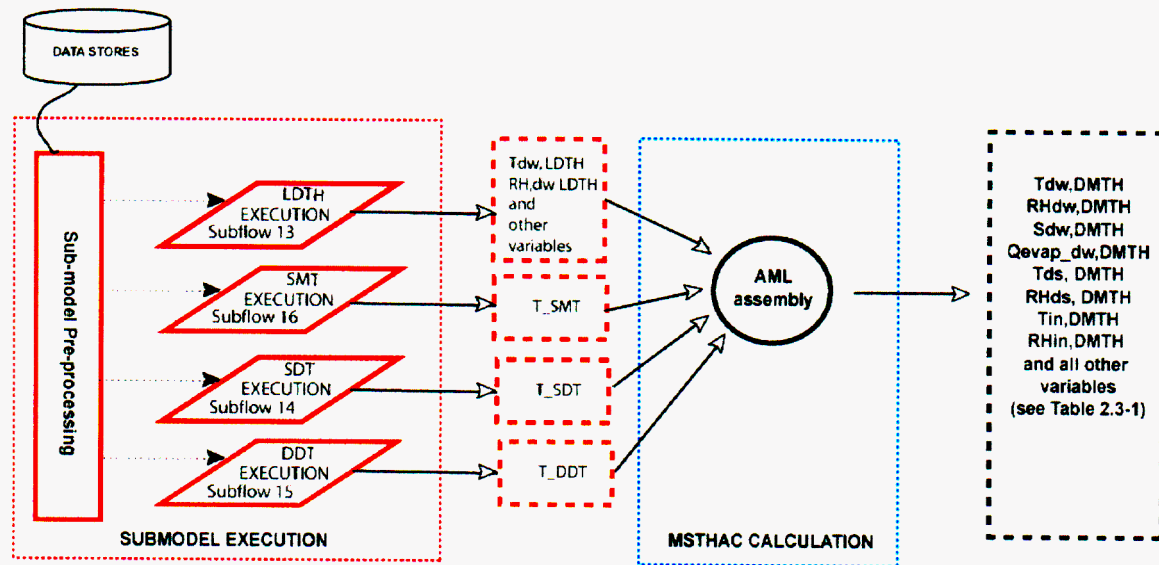


Figure 2. MSTH model flowchart in two steps: (1) NUFT submodel execution in red, and (2) MSTHAC processing of final output (blue).

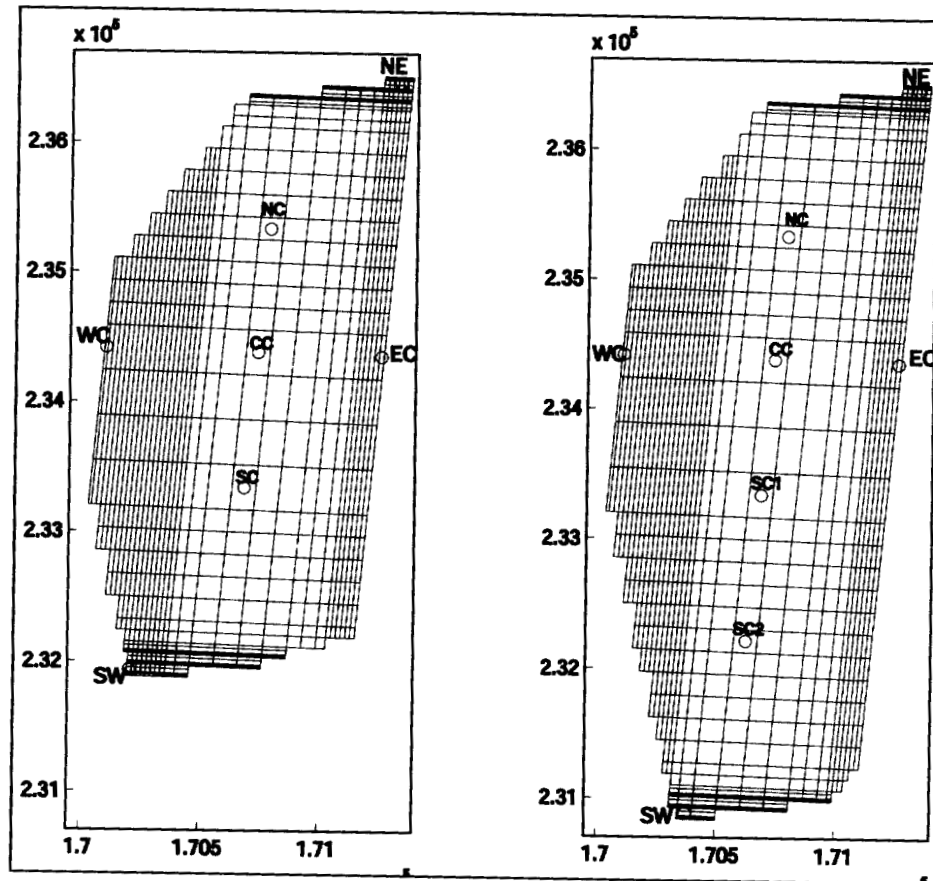


Figure 3. Grid of repository footprint for the HTOM (left) and LTOM (right) operation modes.

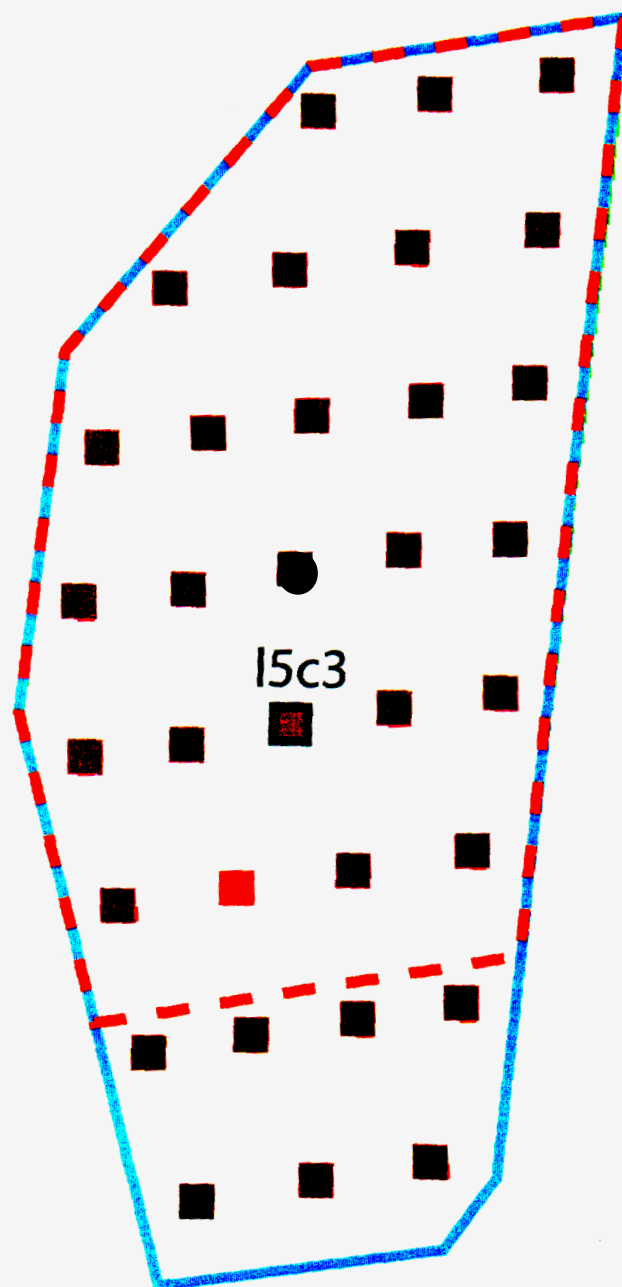
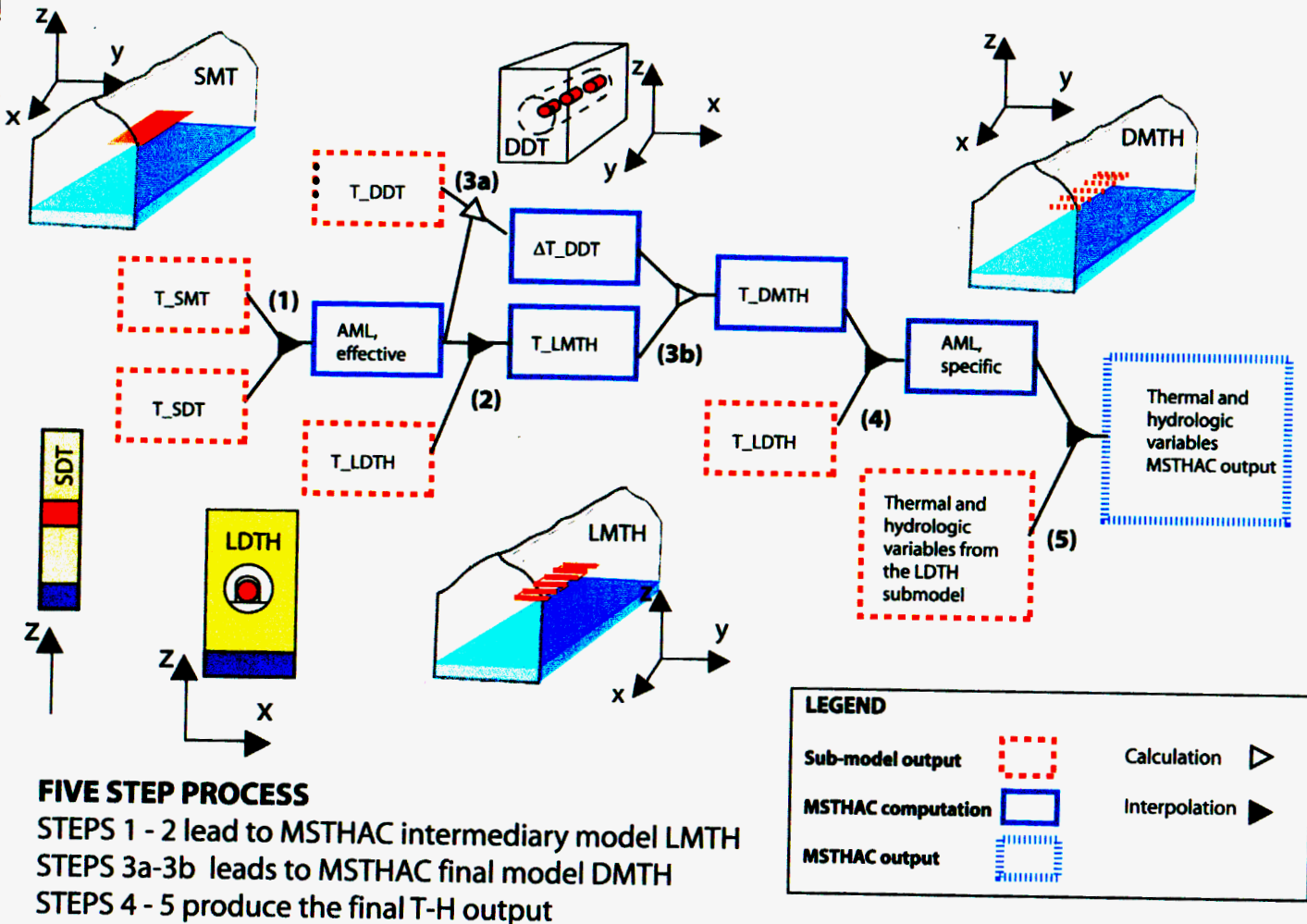


Figure 4. LDTH/SDT calculation locations (total of 33) for the HTOM (red dashed line) and the LTOM (blue solid lines) operation modes.

Figure 5. MSTHAC Five-step Process for each spatial location.



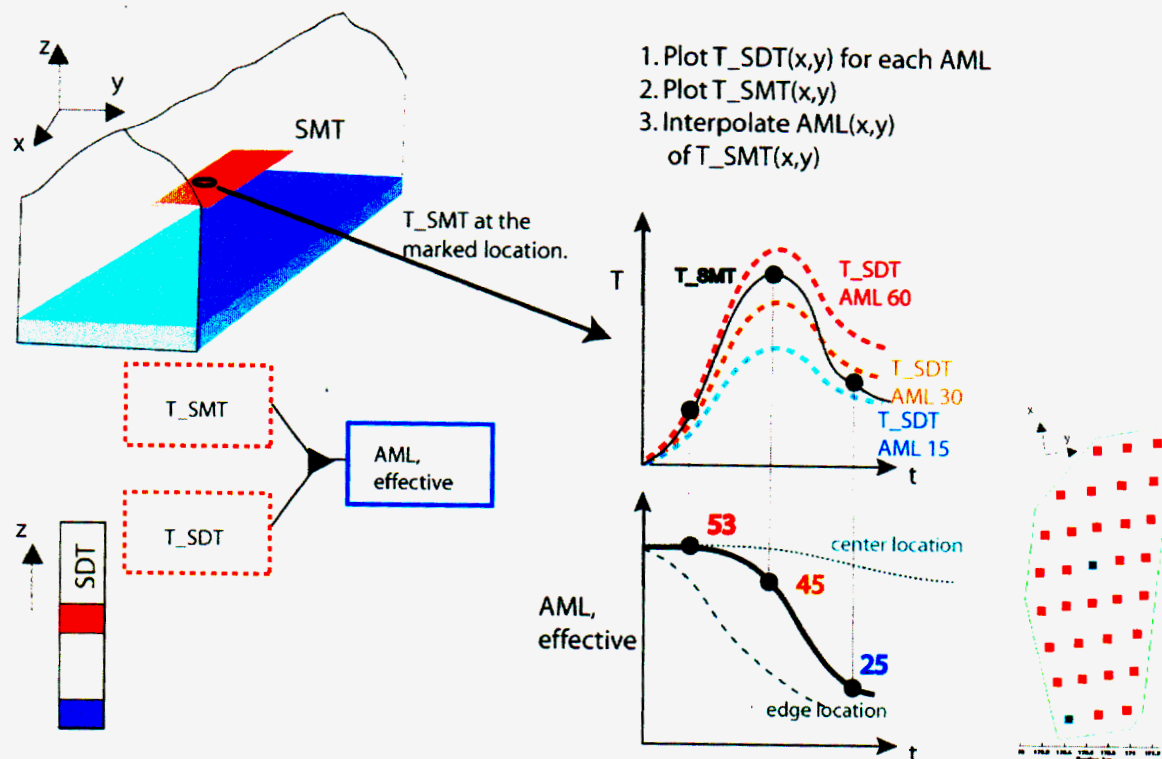


Figure 6. MSTHAC Step 1: interpolation of AML effective from T_SMT and T_SDT .

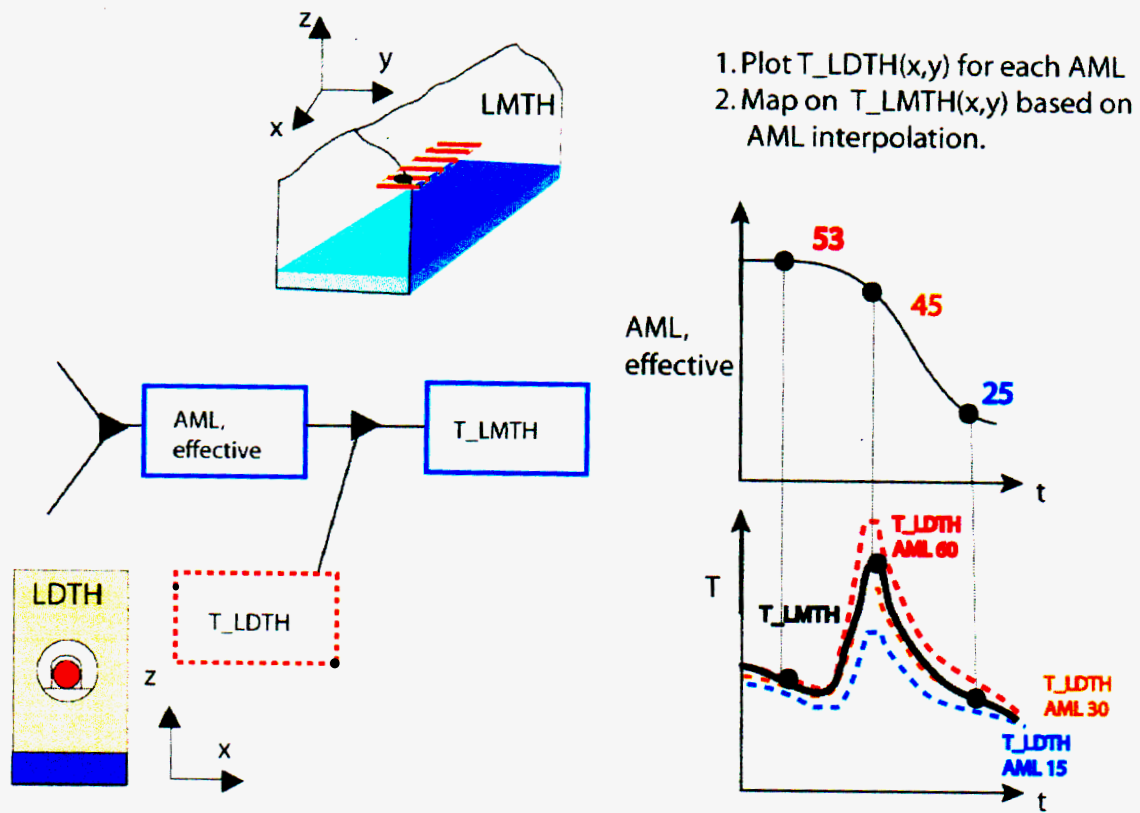


Figure 7. MSTHAC Step 2: interpolation of T_{LMTH} from $AML_{effective}$ and T_{LDTH} .

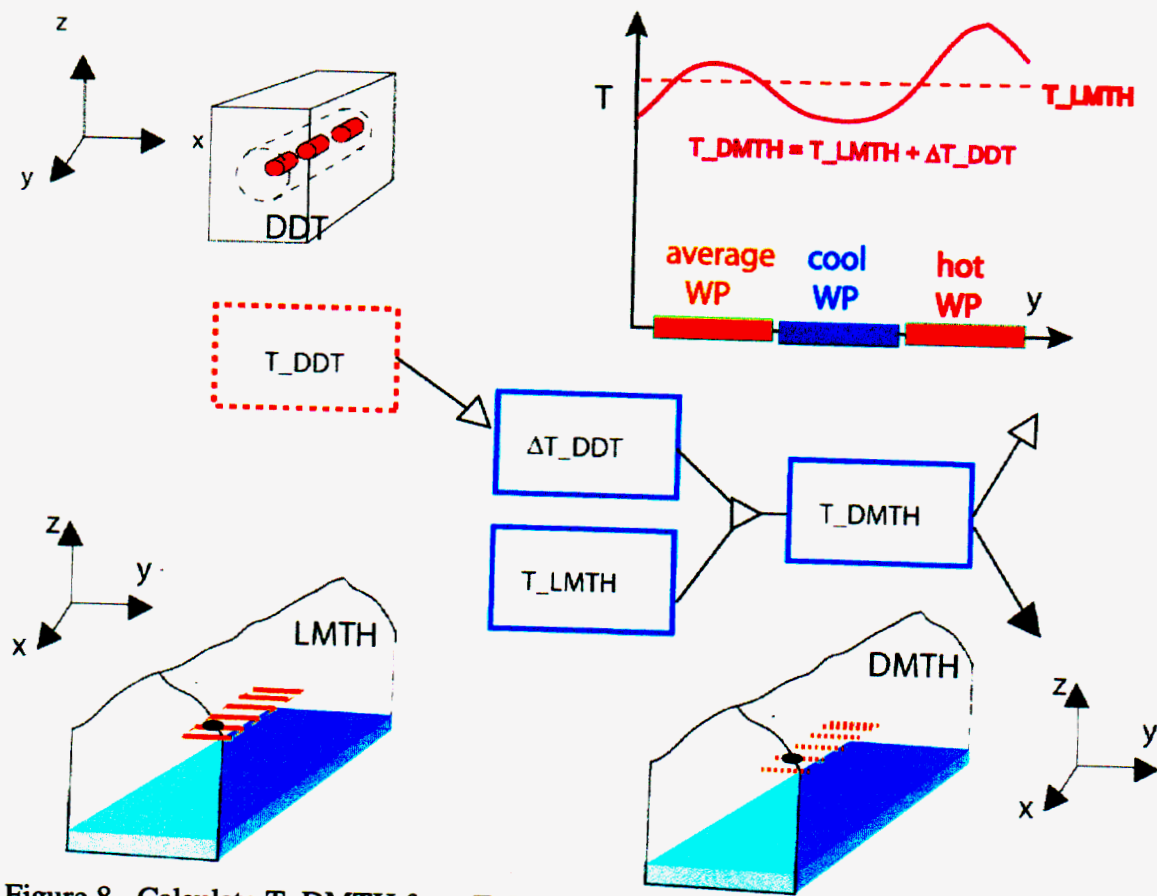


Figure 8. Calculate T_{DMTH} from T_{LMTH} and T_{DDT} .

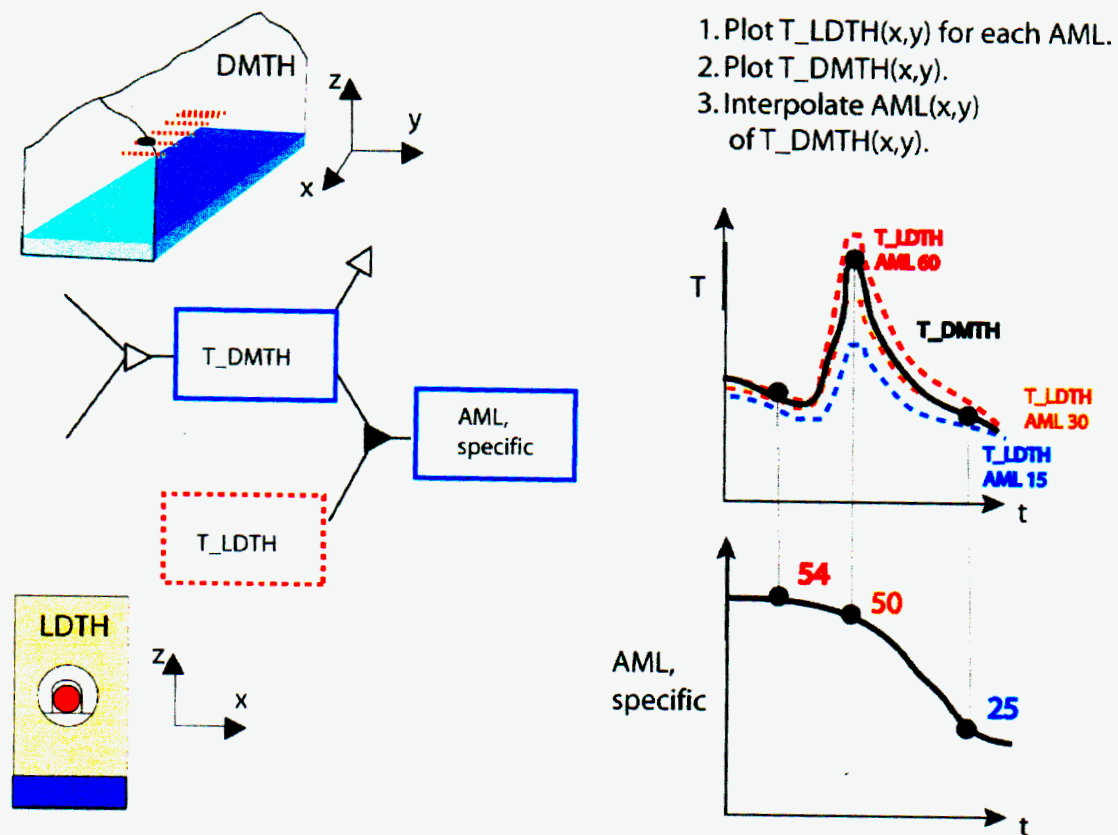


Figure 9. MSTHAC Step 4: interpolate AMLspecific from T_DMTH and T_LDTH.

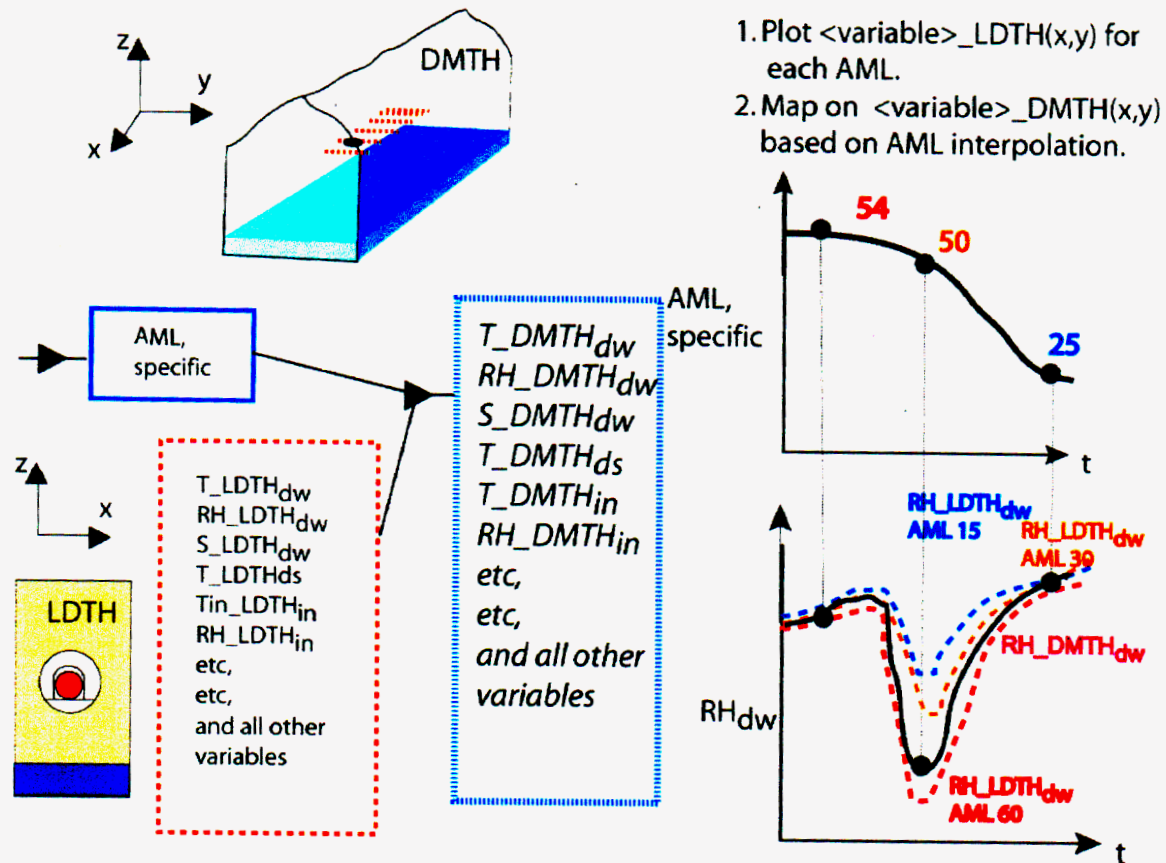


Figure 10. MSTHAC Step 5: Determine MSTHAC output variables for each thermohydrologic variable from AMLspecific and the variables value as computed in the LDTH submodel.

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